

FIG. 1(a)

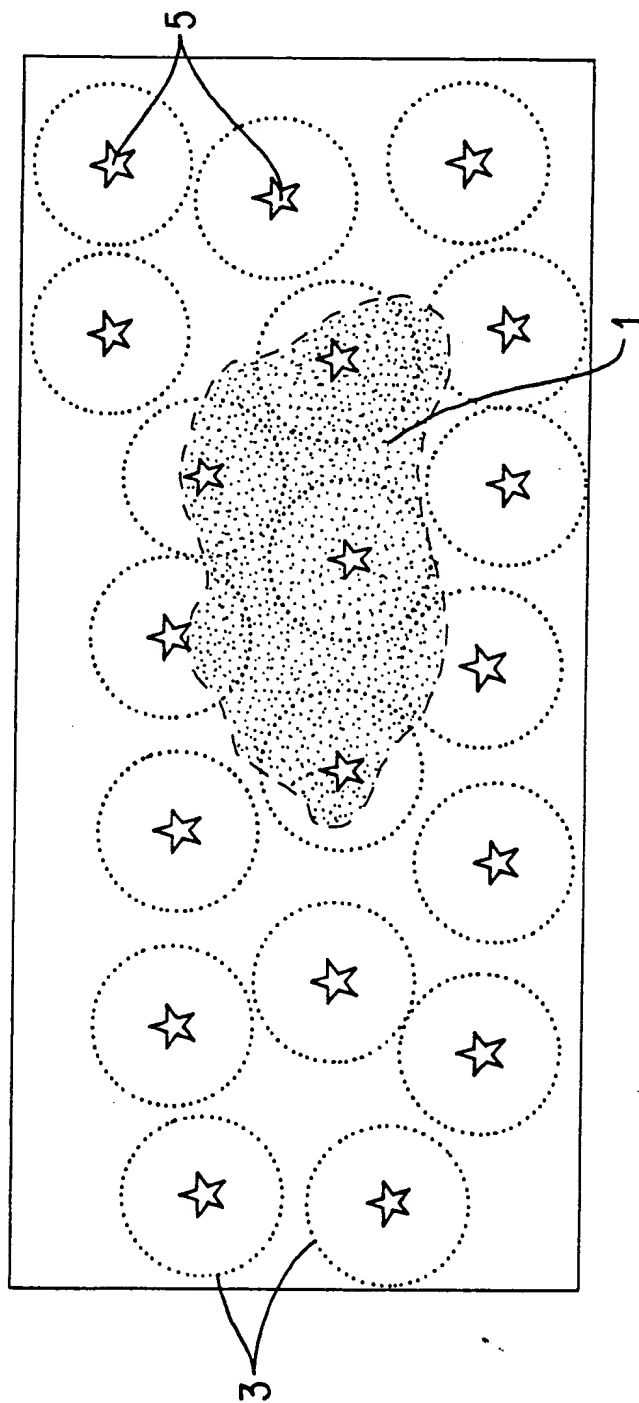


FIG. 1(b)

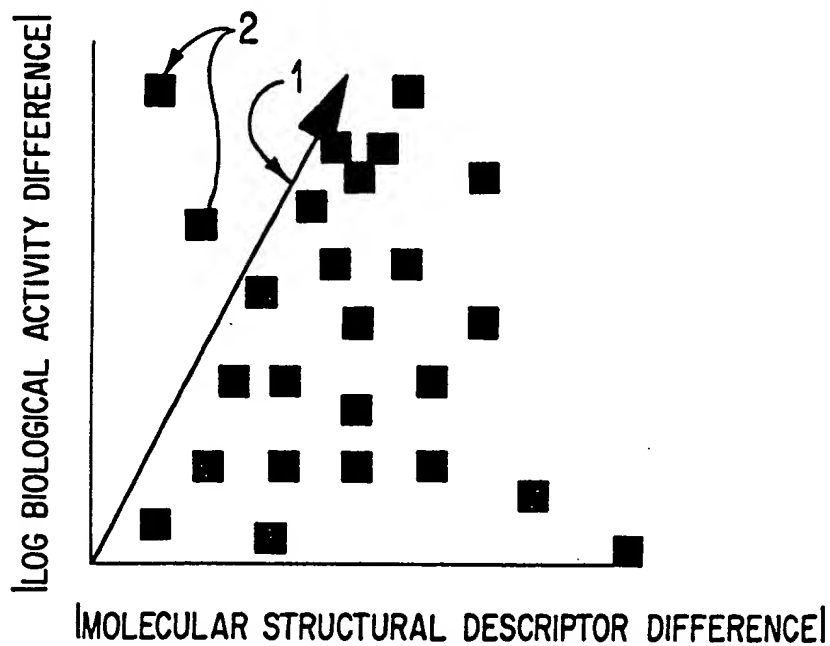


FIG. 2

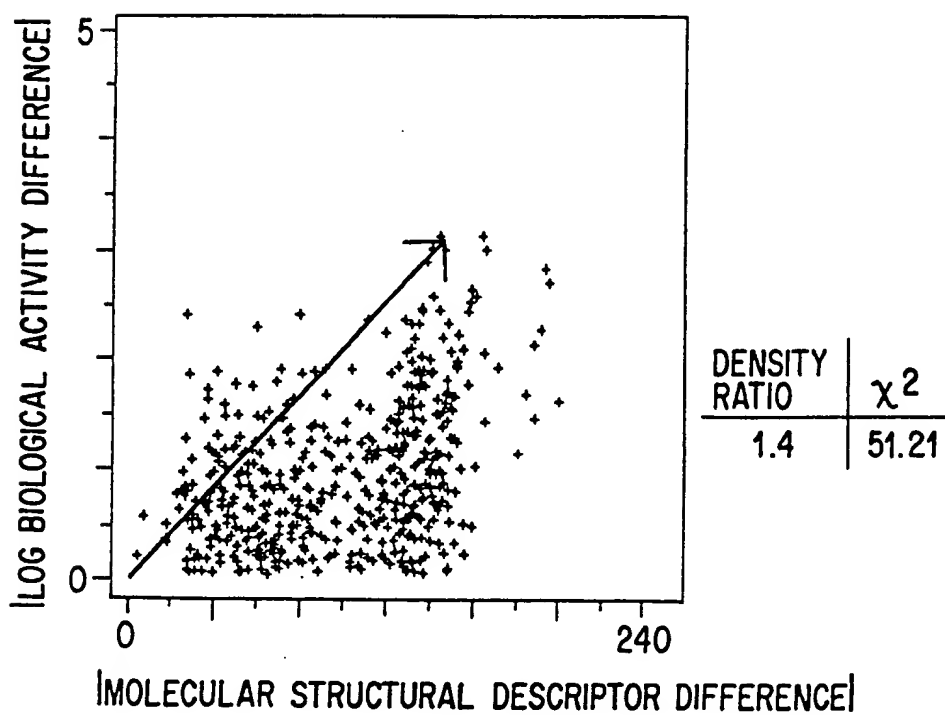


FIG. 3

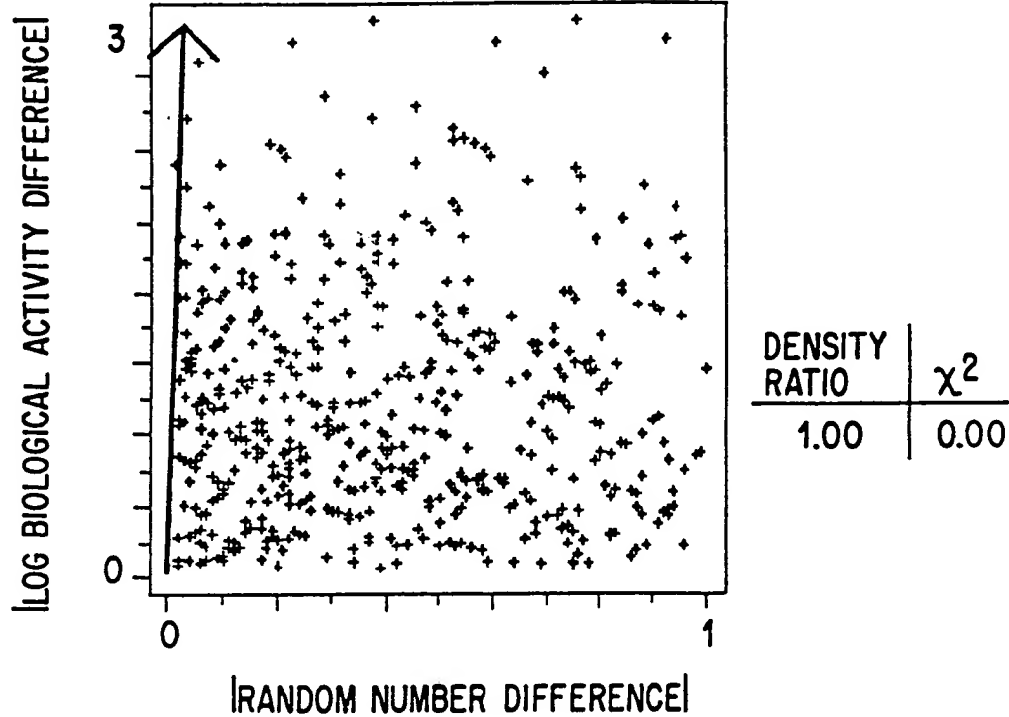


FIG. 4

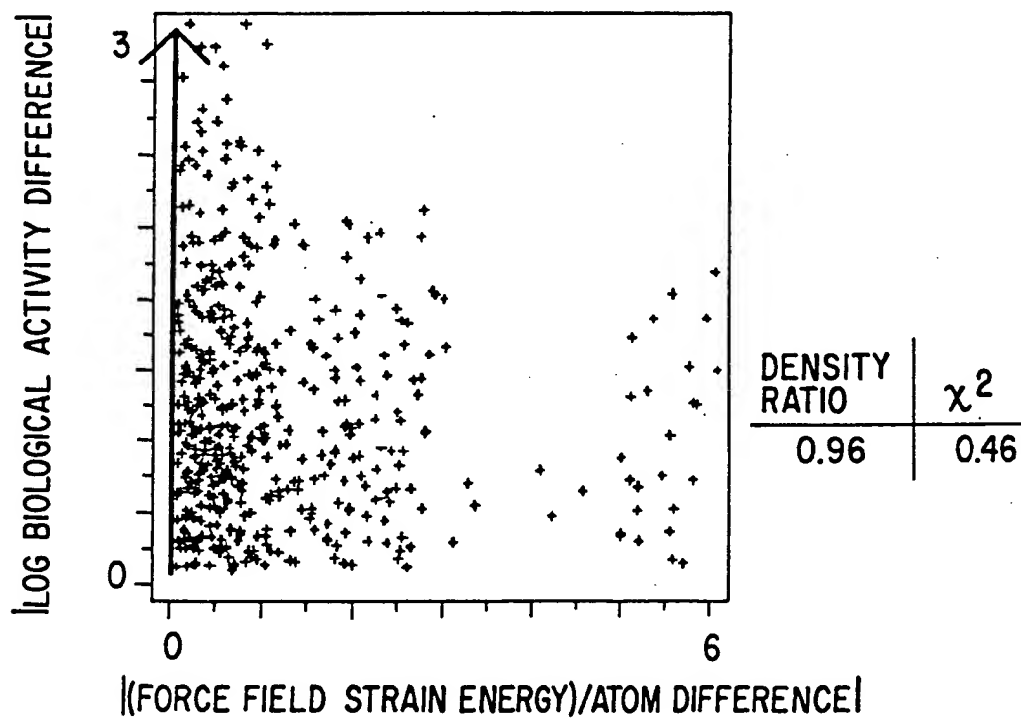
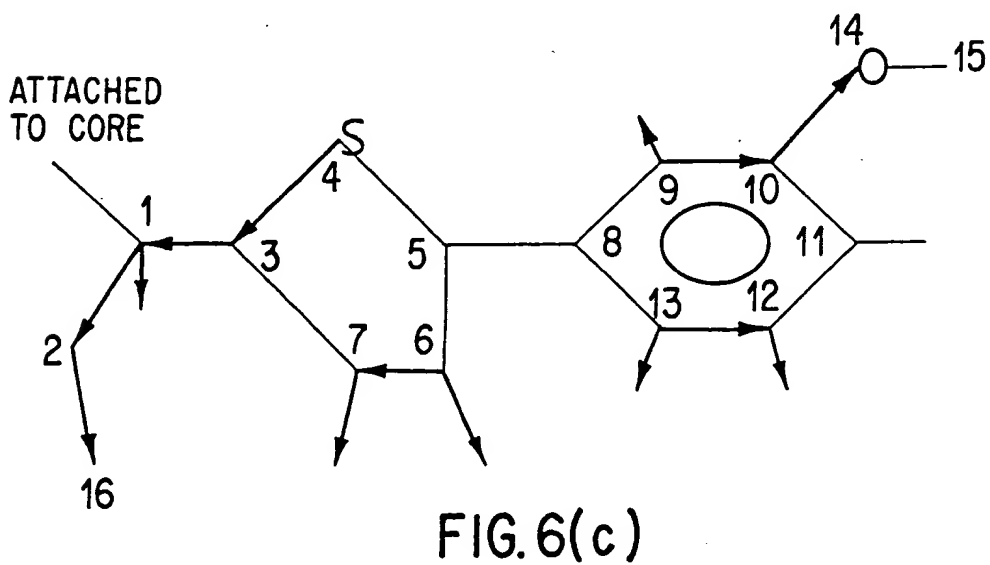
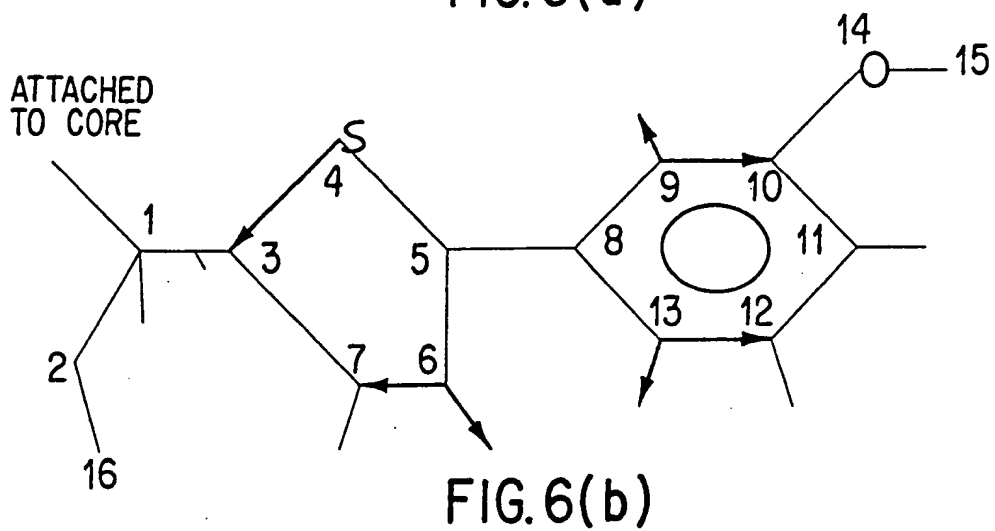
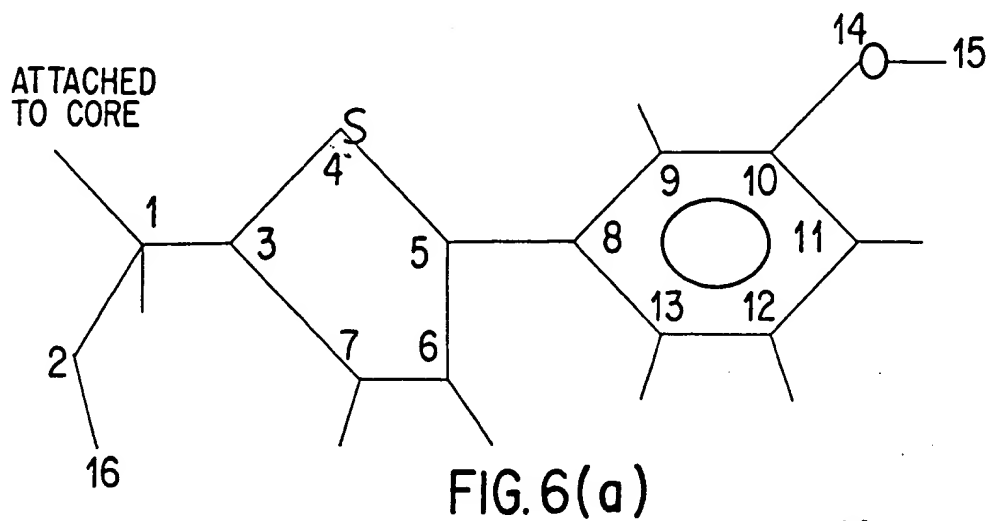


FIG. 5



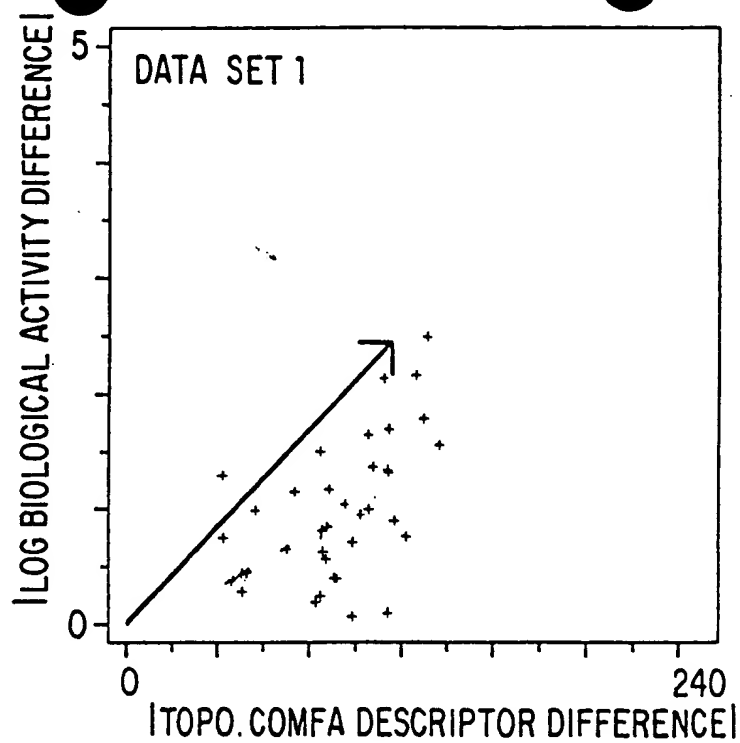


FIG.7(a)

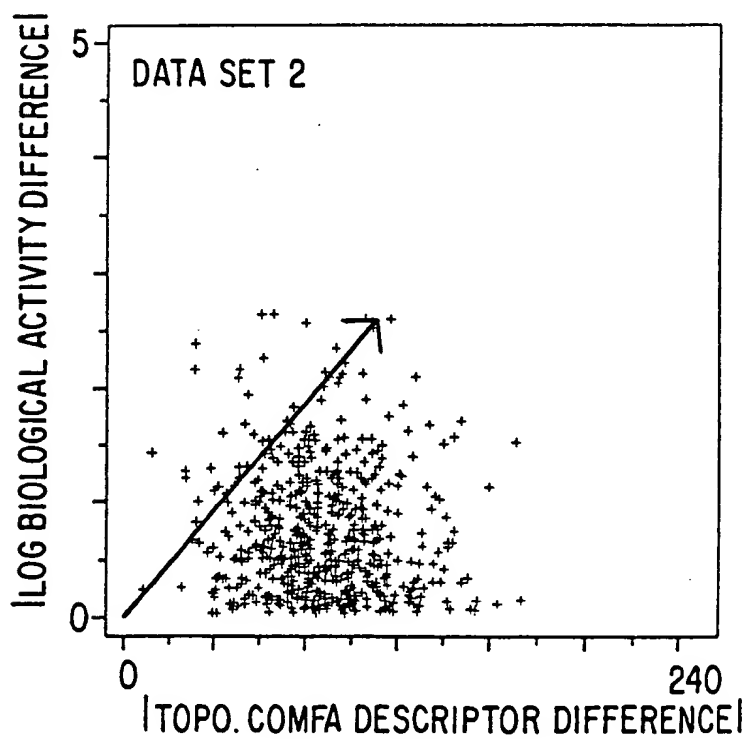


FIG.7(b)

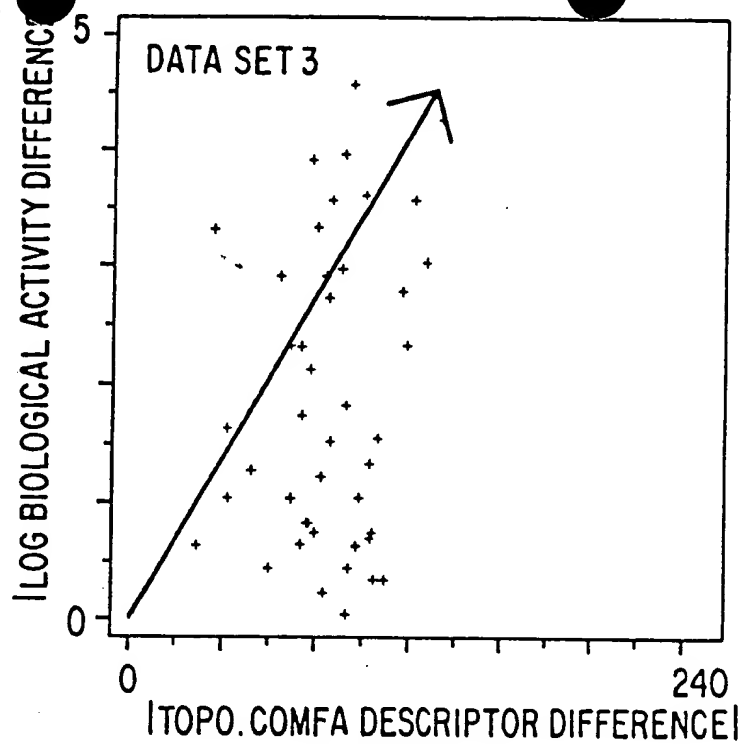


FIG. 7(c)

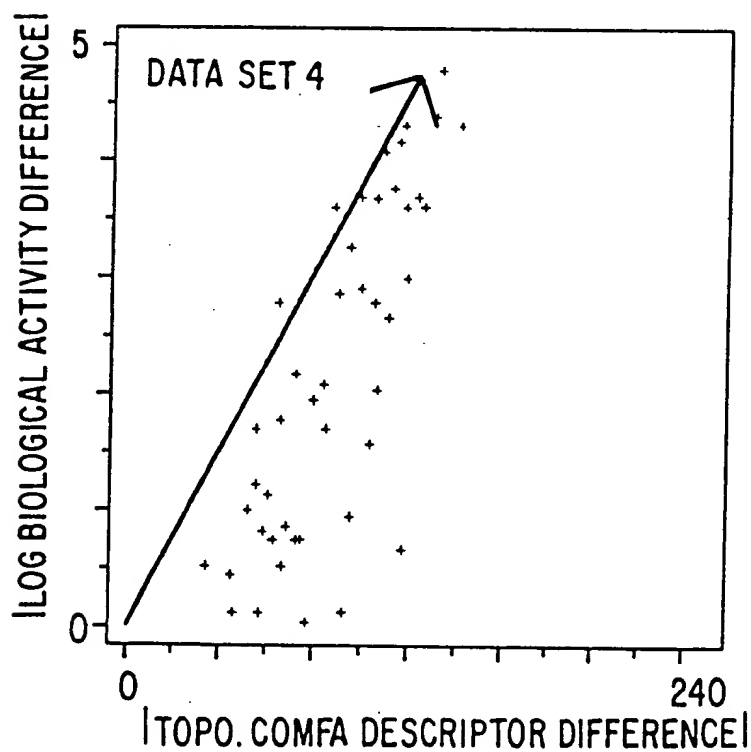


FIG. 7(d)

TOPOL 3029460

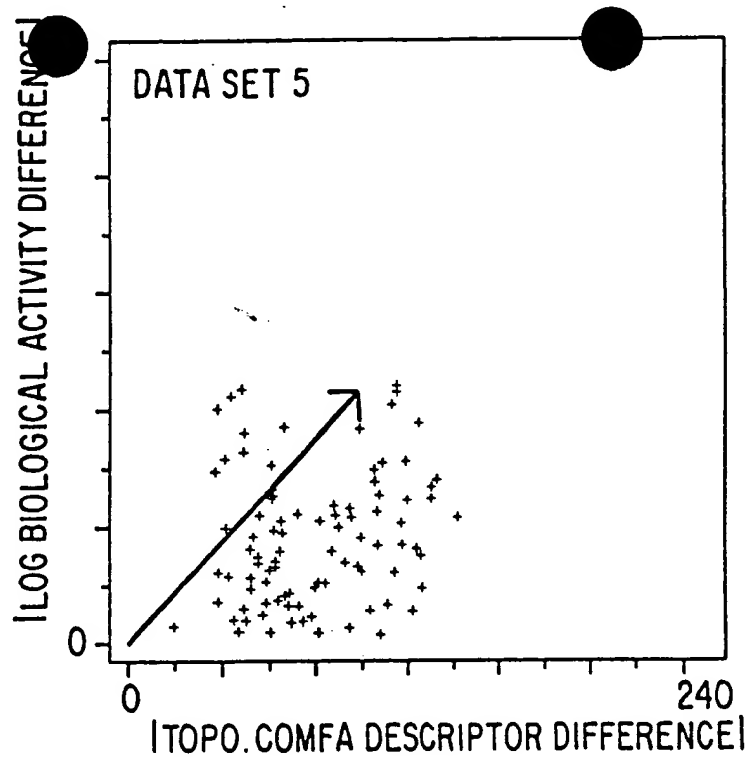


FIG.7(e)

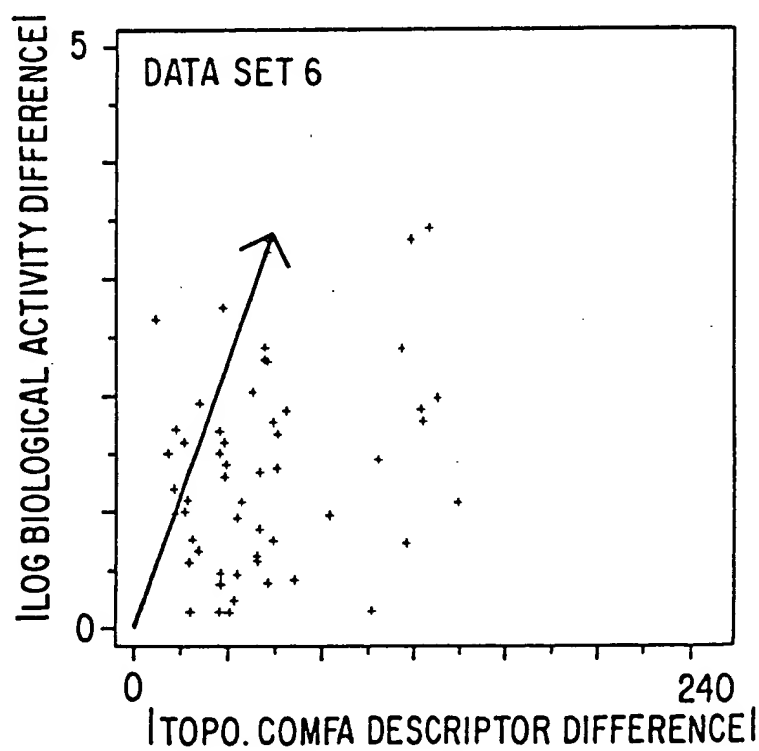


FIG.7(f)



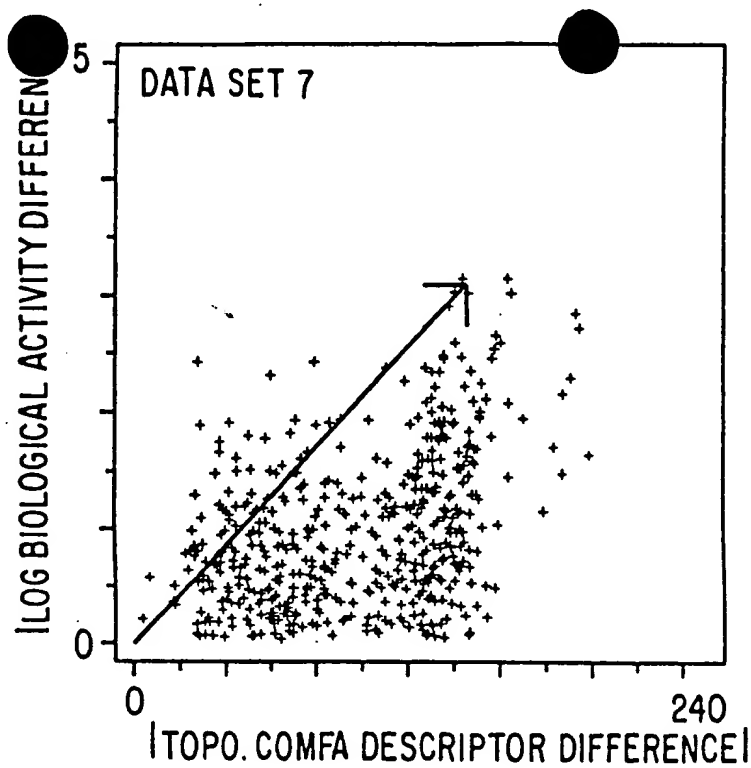


FIG.7(g)

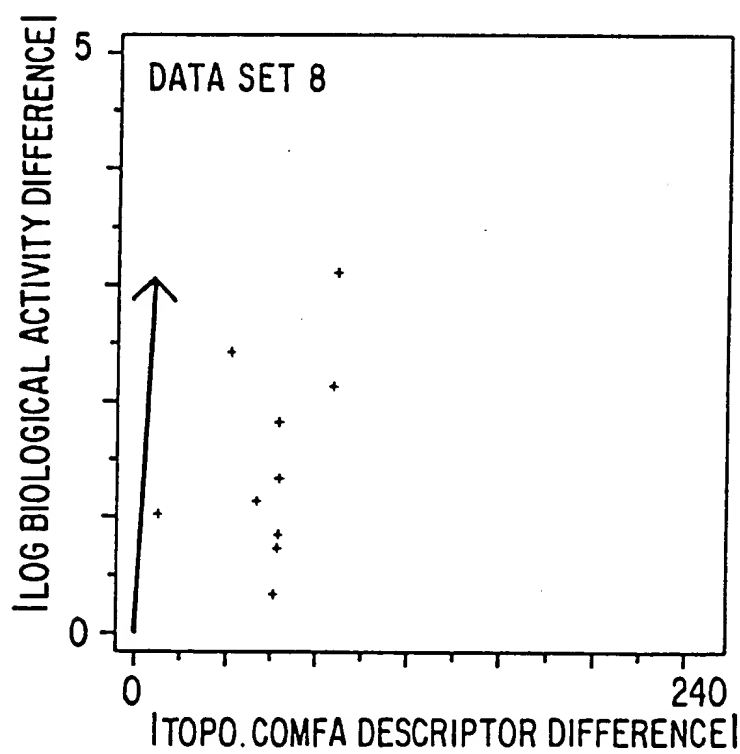


FIG.7(h)

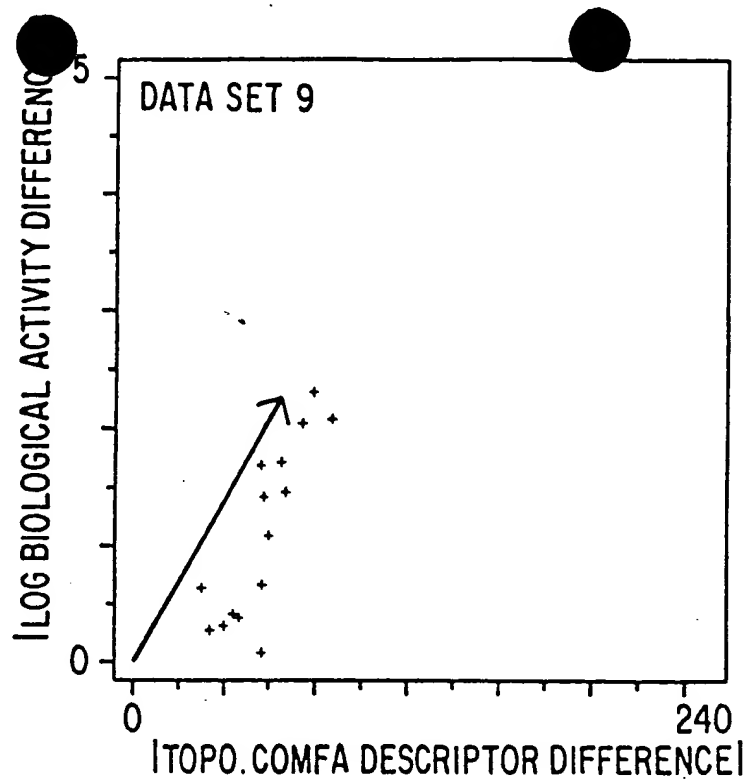


FIG.7(i)

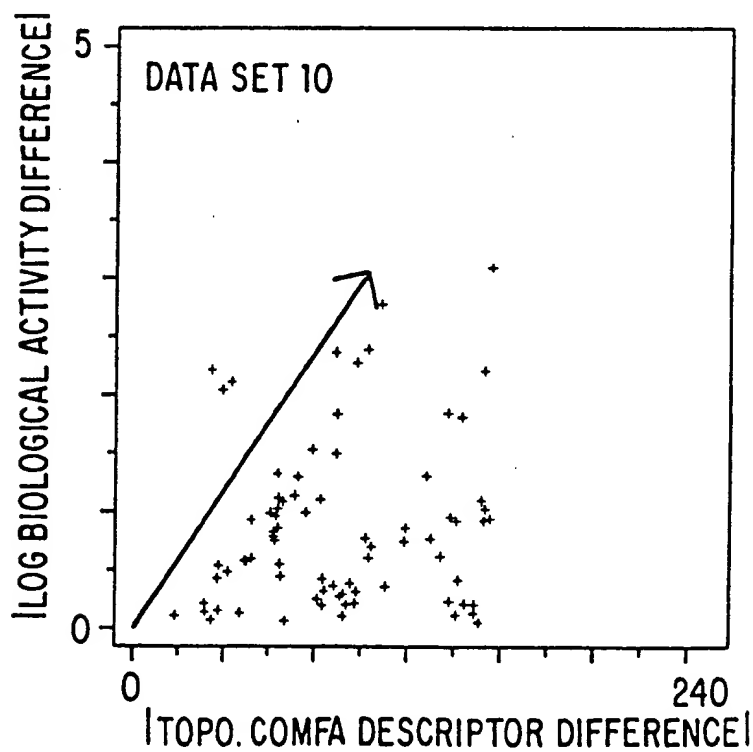


FIG.7(j)

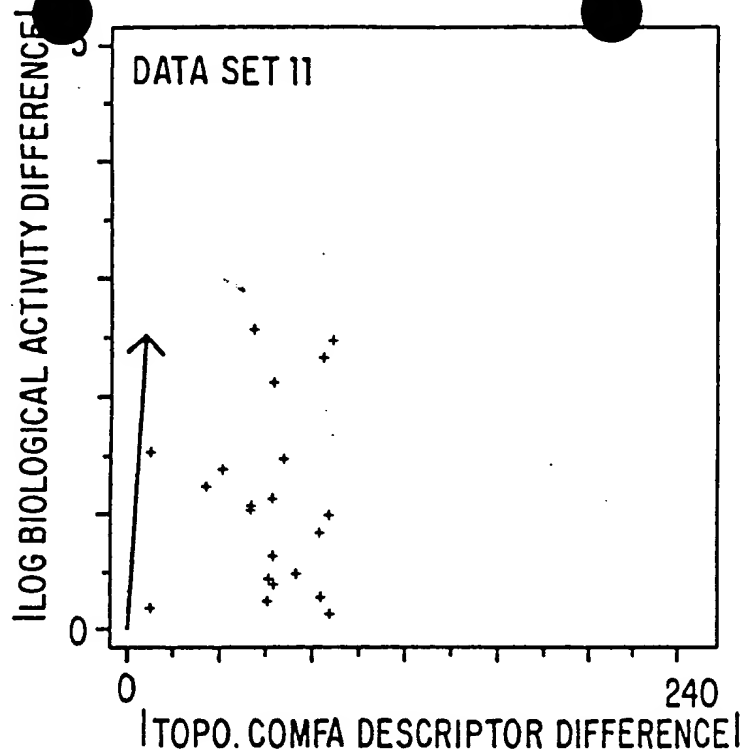


FIG.7(k)

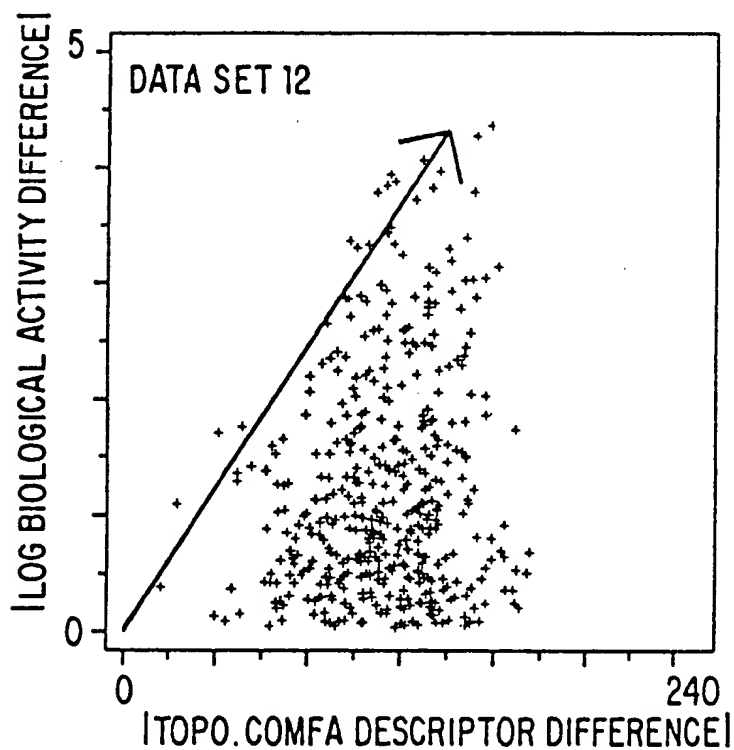


FIG.7(l)

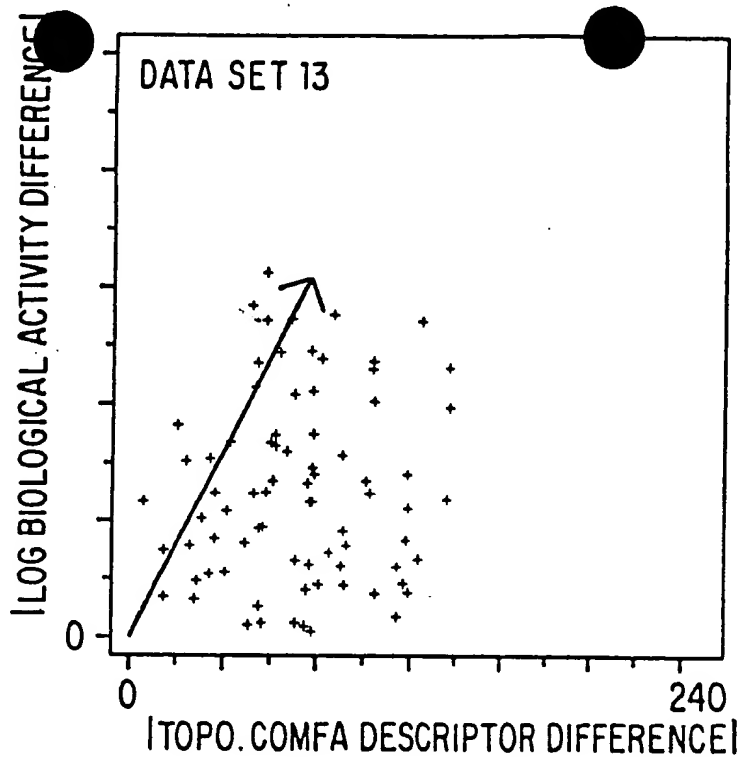


FIG.7(m)

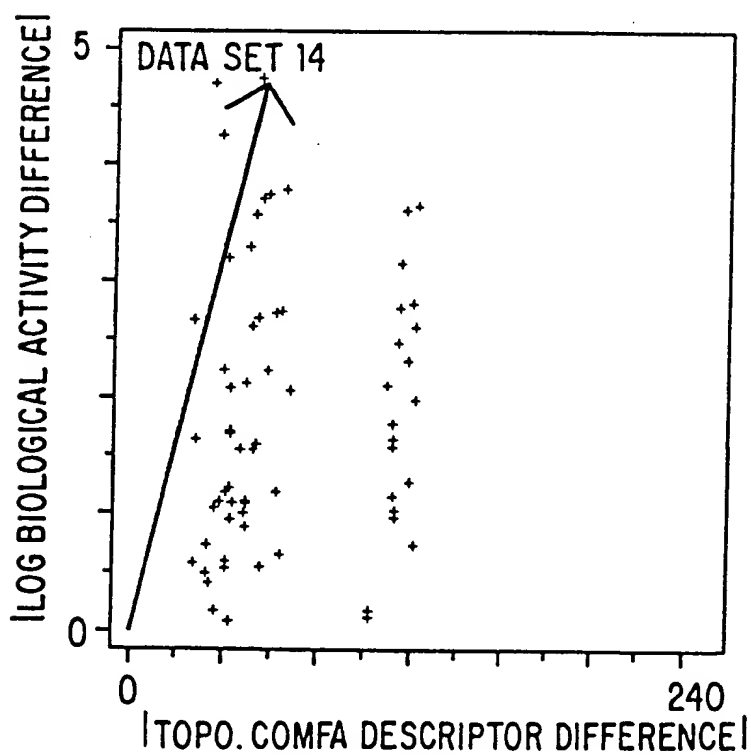


FIG.7(n)

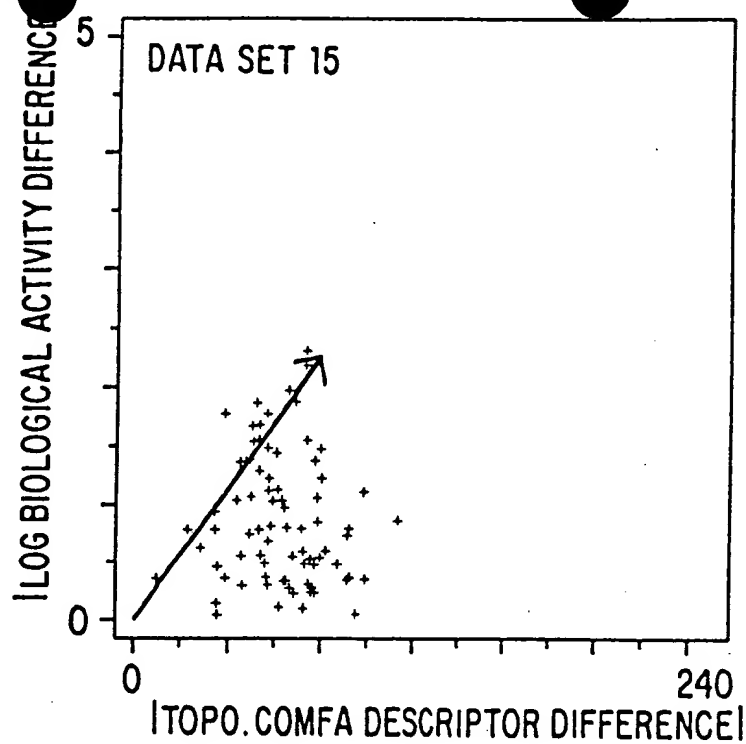


FIG.7(o)

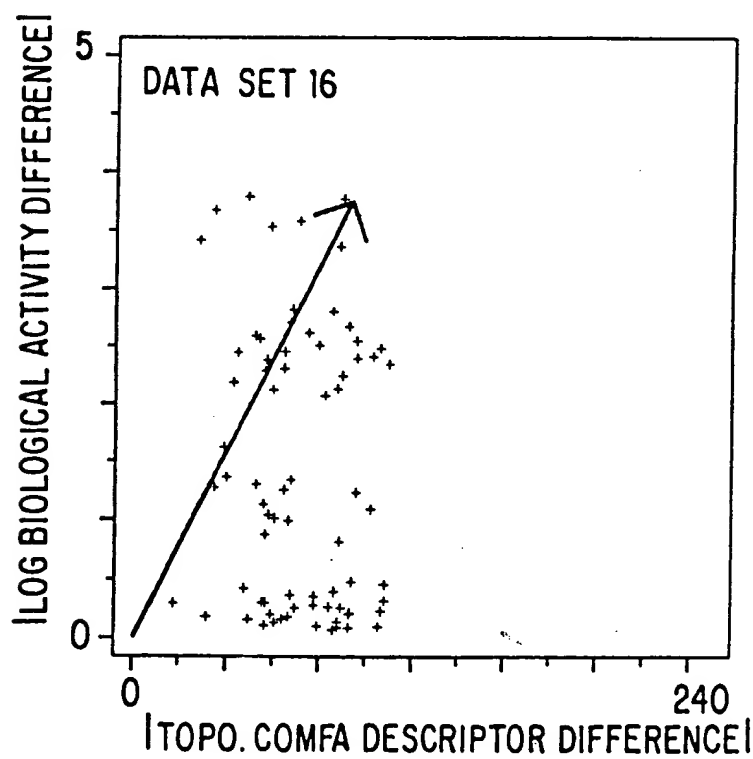


FIG.7(p)

FO5020" 80294460

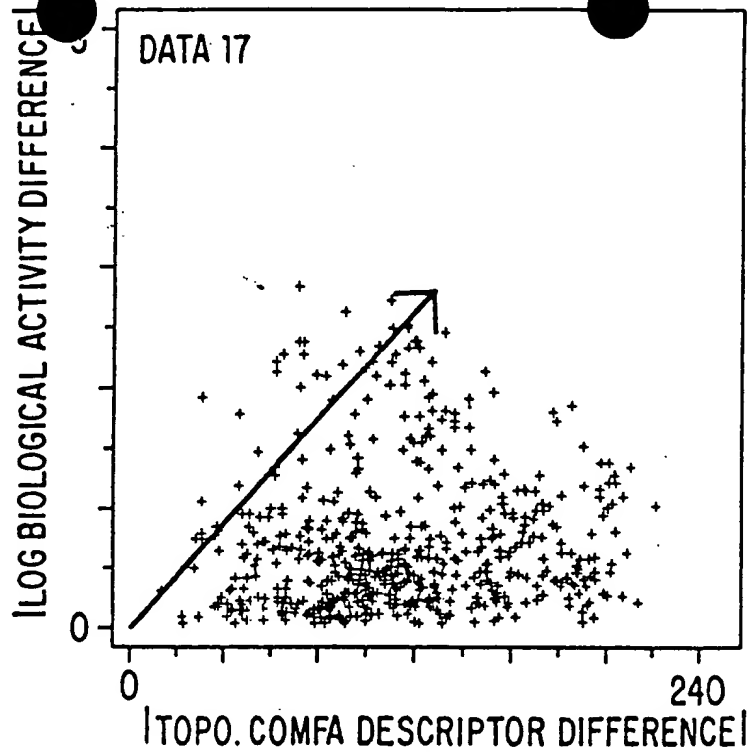


FIG.7(q)

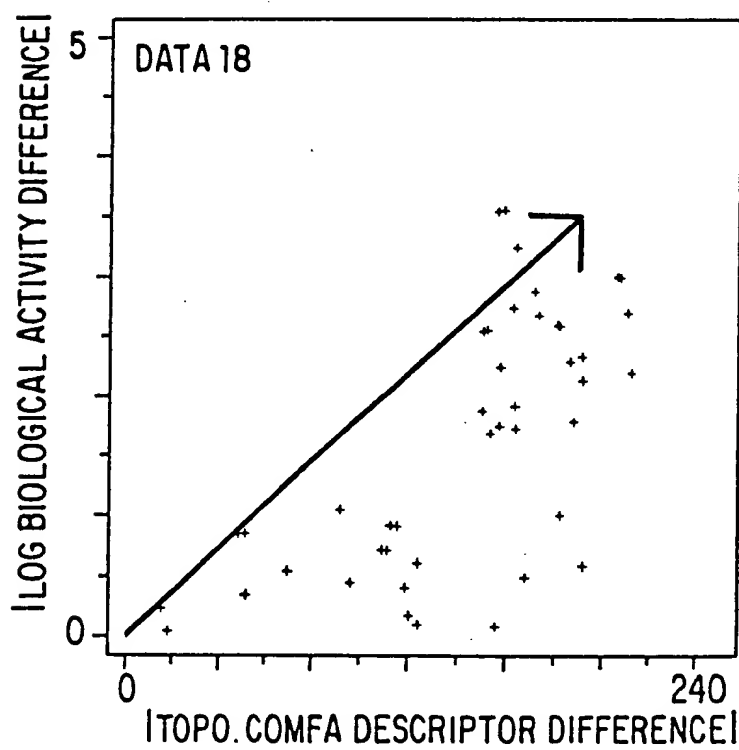


FIG.7(r)

FOUO 8029260

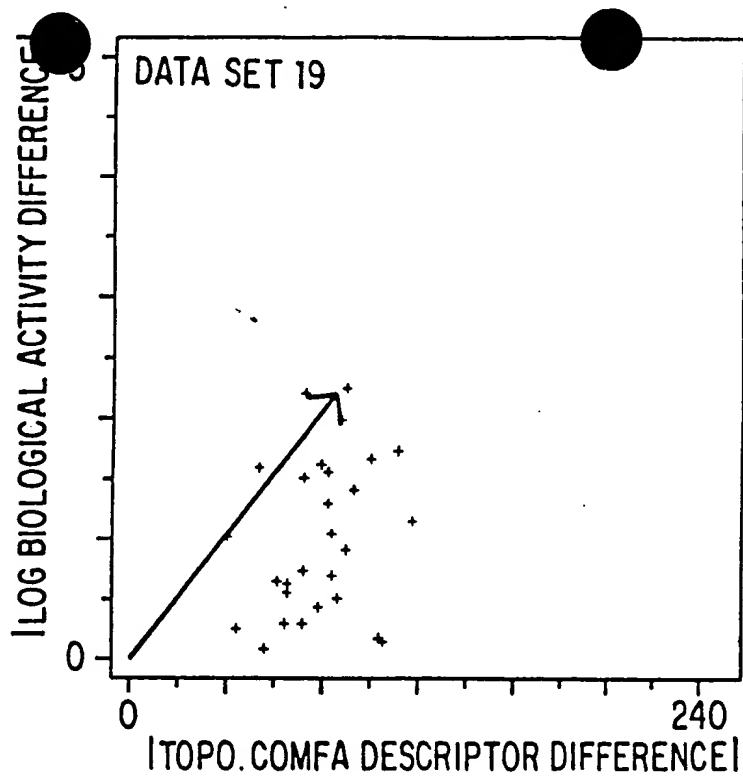


FIG.7(s)

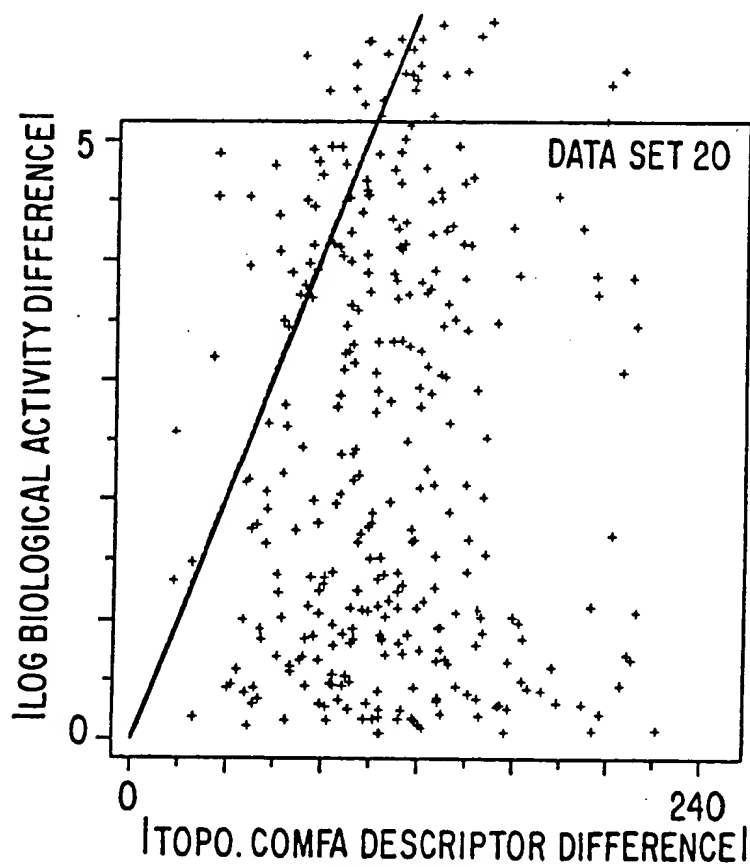
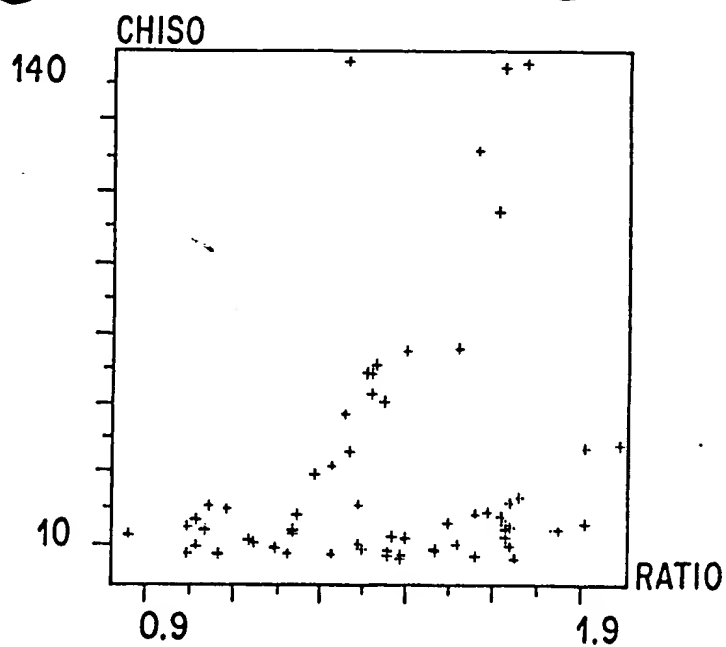


FIG.7(t)

105020" 80292260



1.1

FIG. 8(a)

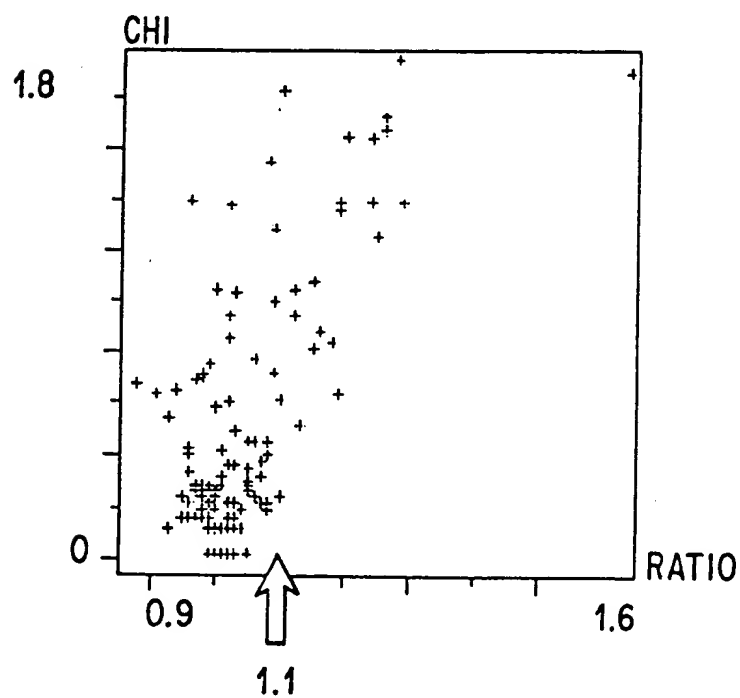


FIG. 8(b)



FO5020" 30494260

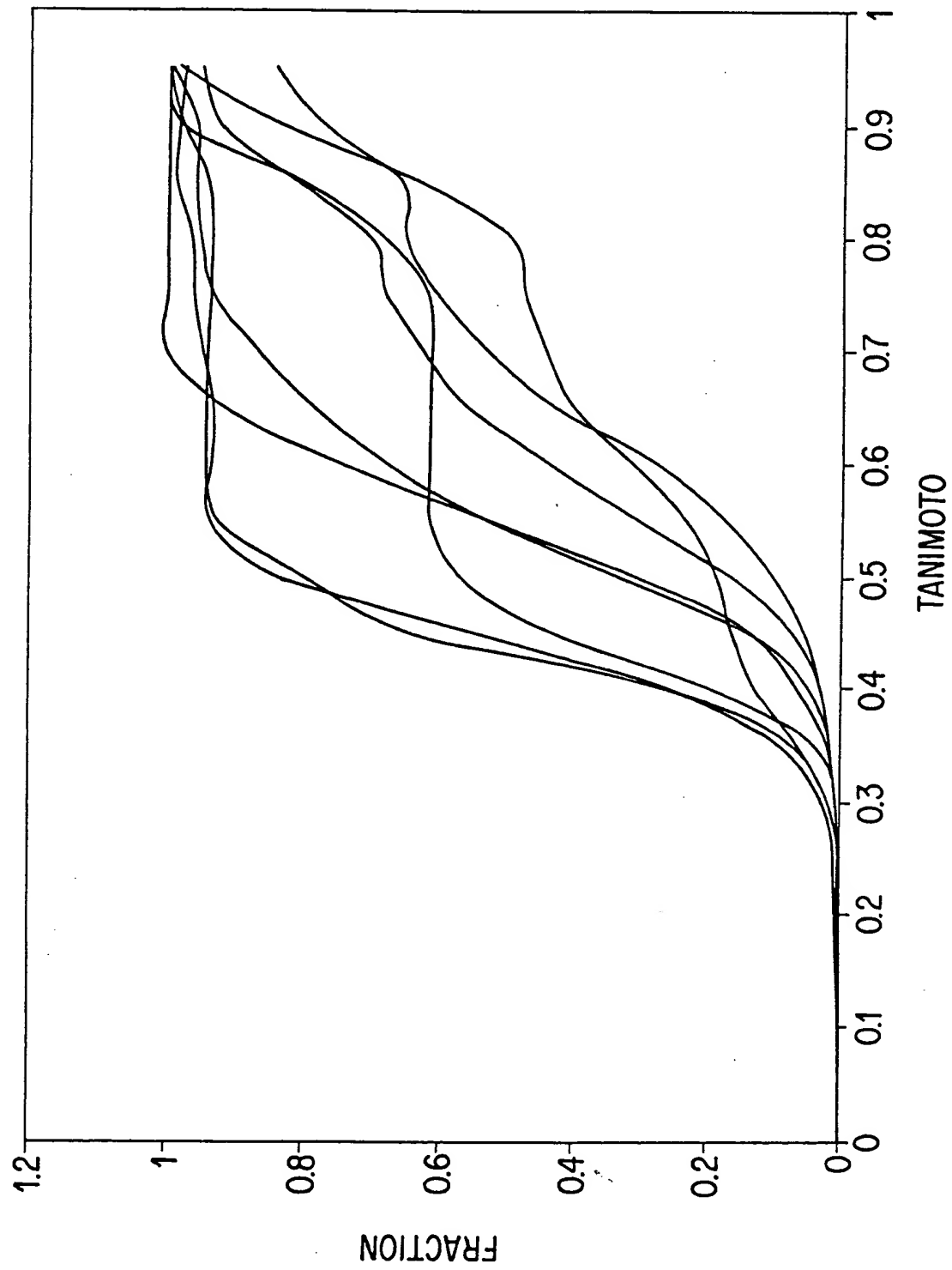


FIG. 9(a)

FO9020" 80292260

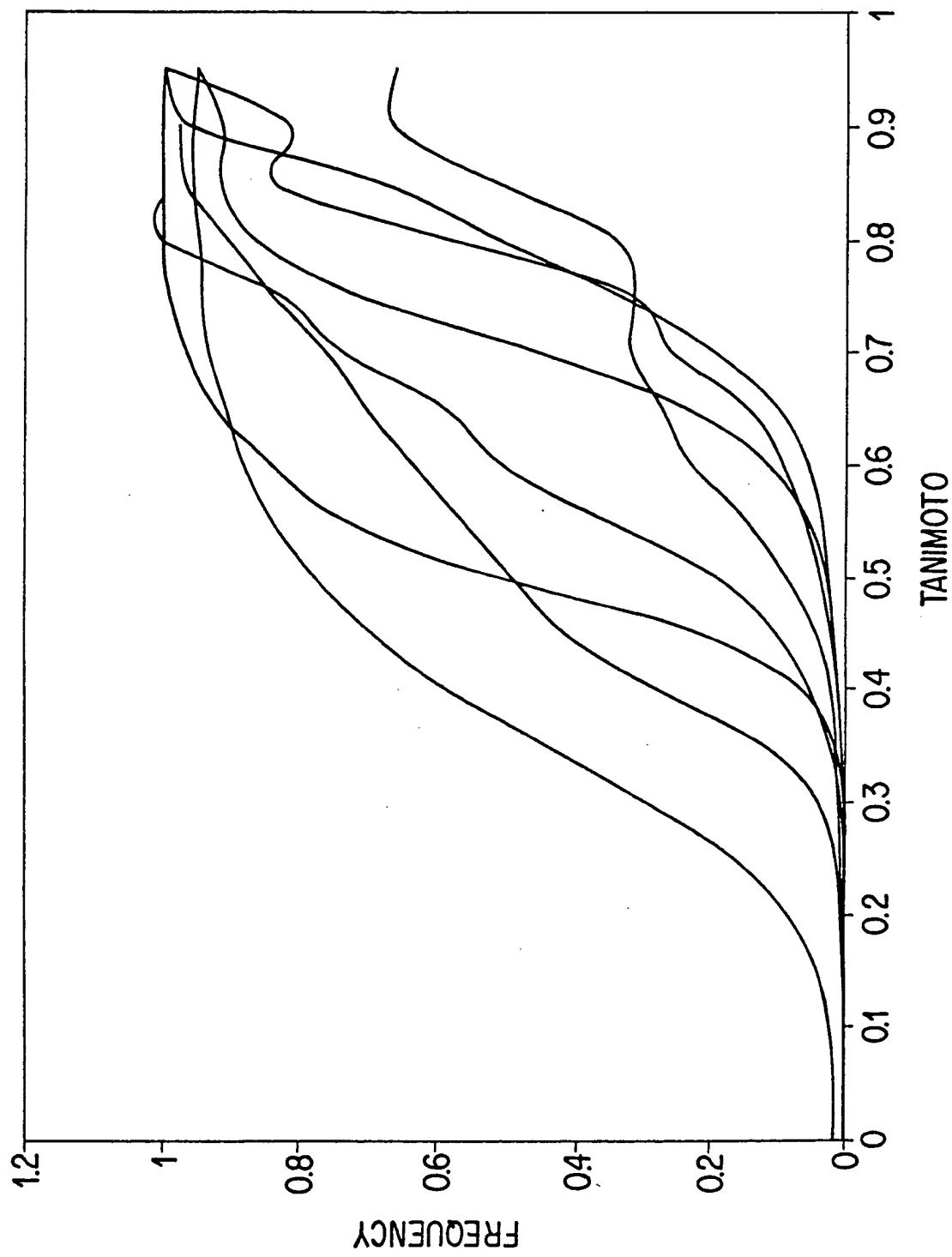


FIG. 9(b)

FOUO 3029260

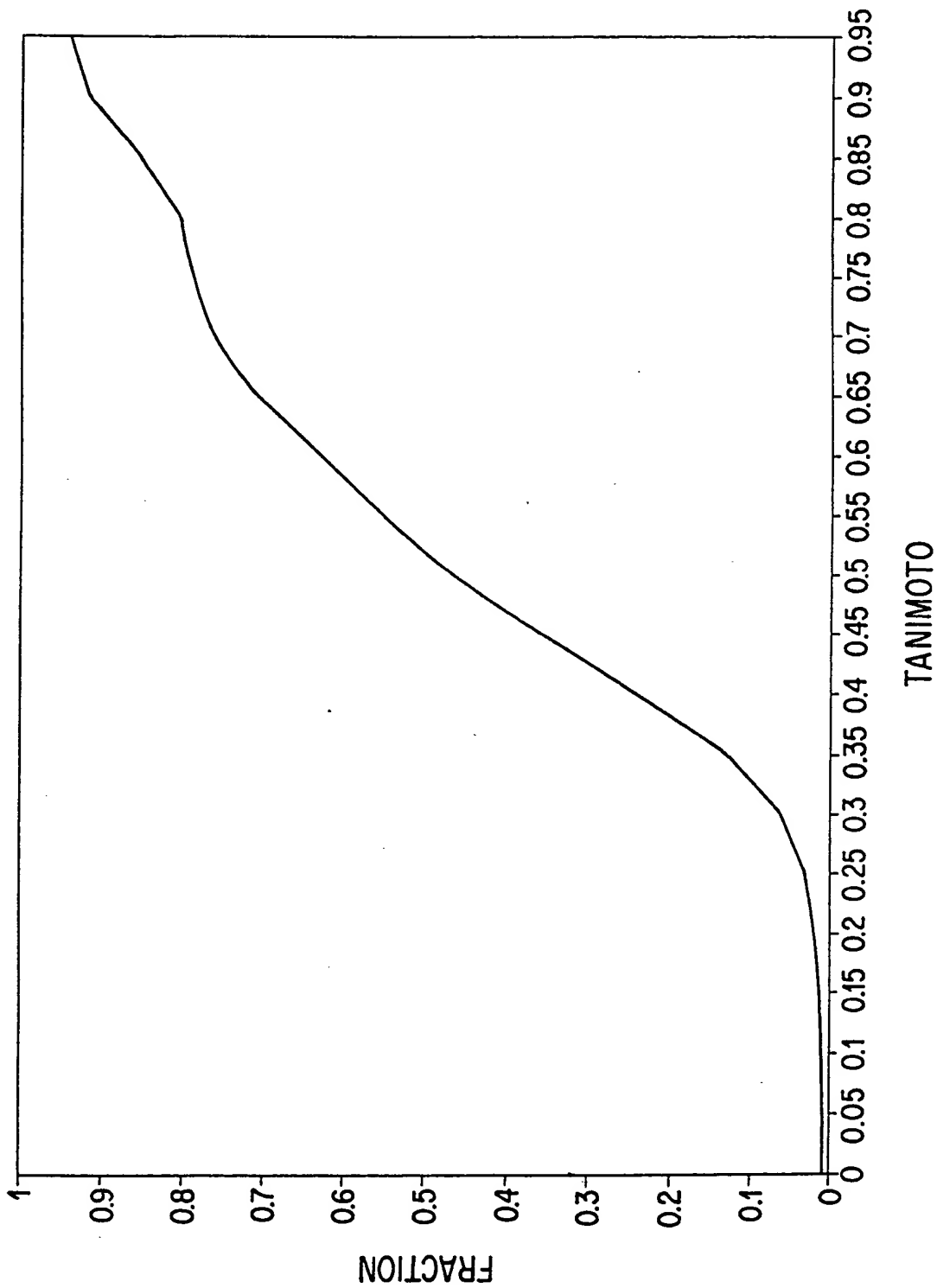


FIG. 9(c)

FIG. 10(a)

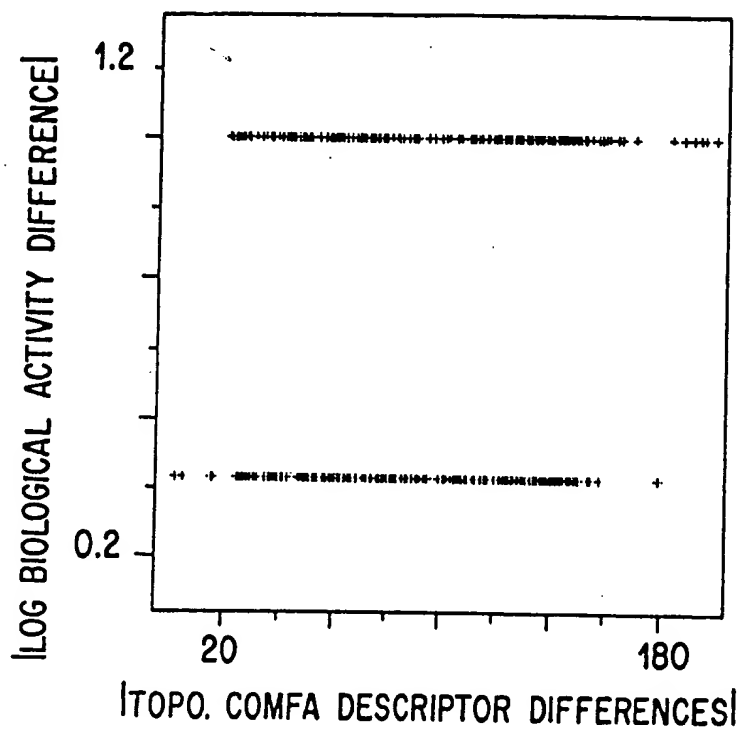


FIG.10(a)

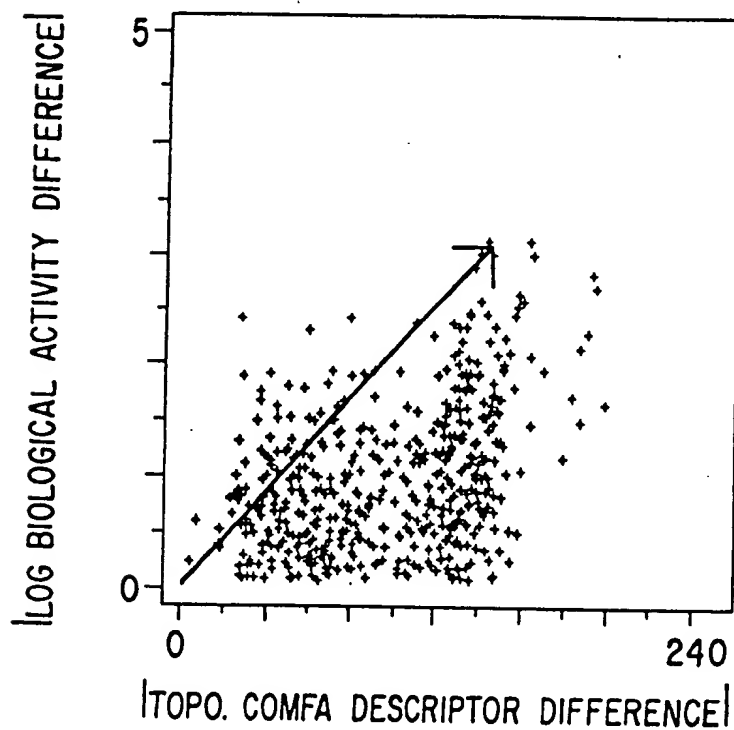


FIG.10(b)

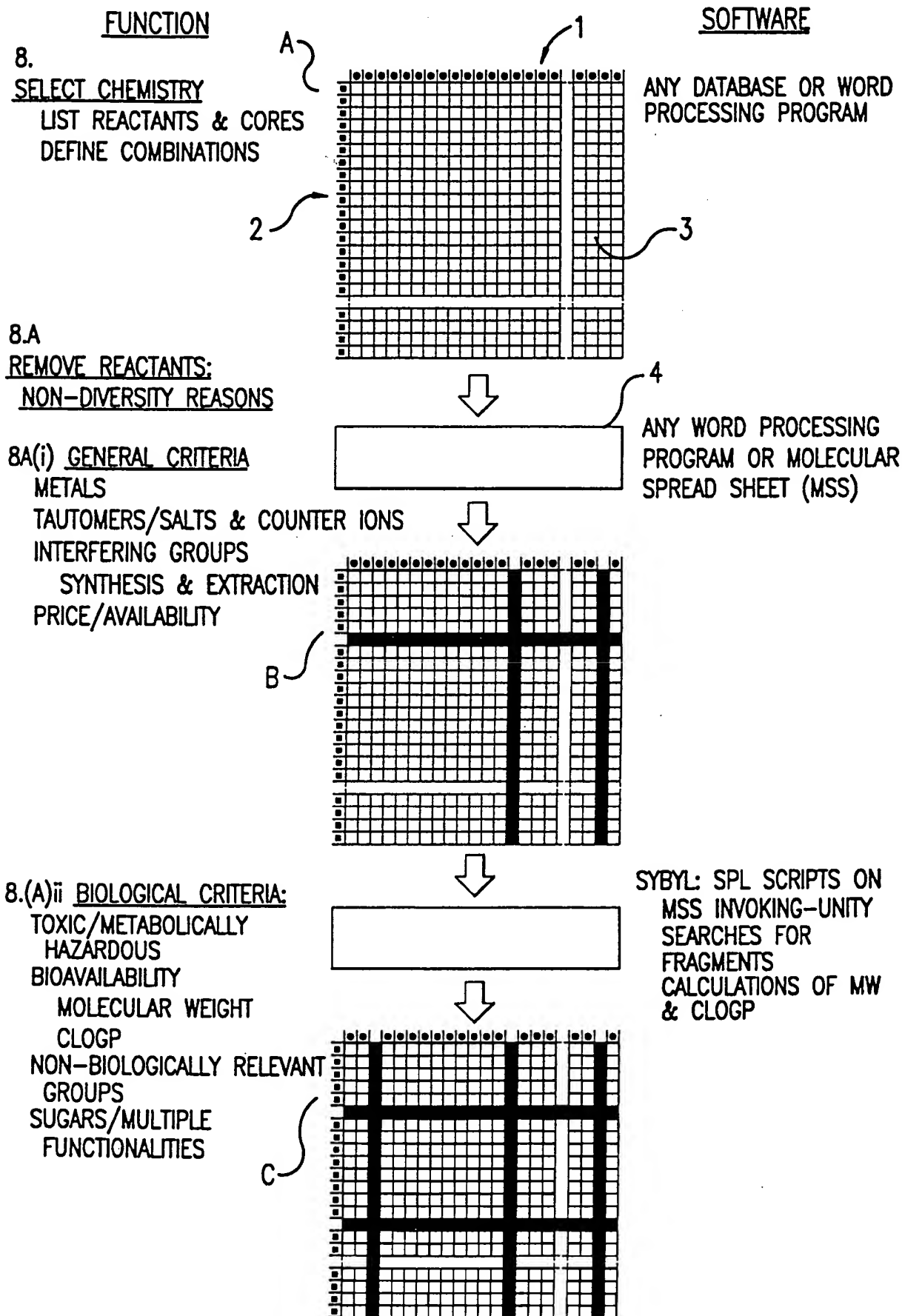


FIG.11(a)

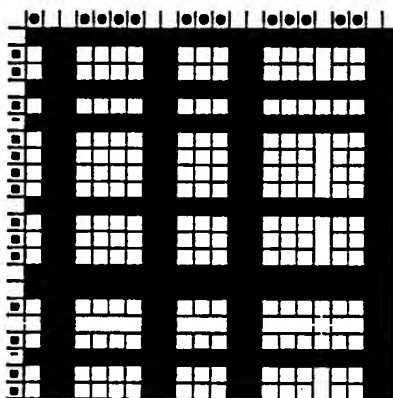
8B

REMOVE NON-DIVERSE REACTANTS:

3D STRUCTURE GENERATION  
TOPOMERIC CONFORMER  
ALIGNMENT  
CoMFA FIELD GENERATION:  
HYDROGEN BOND FIELD  
GENERATION  
ROTATABLE BOND FIELD  
ATTENUATION  
CALCULATE FIELD  
DIFFERENCES  
CLUSTER  
REACTANT SELECTION FROM  
EACH CLUSTER

SYBYL: SELECTOR &  
CONCORD 3.2.1  
SPECIALIZED SOFTWARE:  
APPENDIX "A"  
(SYBYL: CoMFA  
STERIC & MSS)

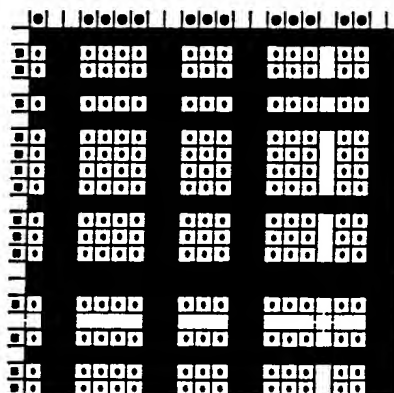
SYBYL: HIERCHICAL  
CLUSTER - MSS  
SYLBL: MSS



8C

COMBINE REACTANTS TO BUILD PRODUCTS

E



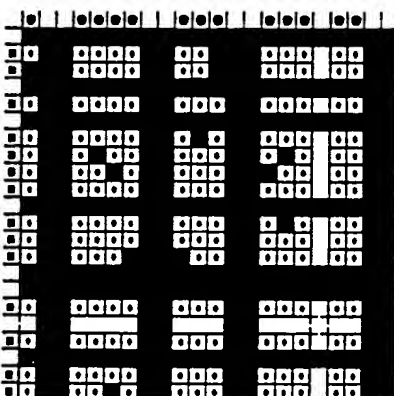
SYBYL: LEGION MSS

8D

REMOVE PRODUCTS:  
NON-DIVERSITY REASONS

GENERAL CRITERIA:

F



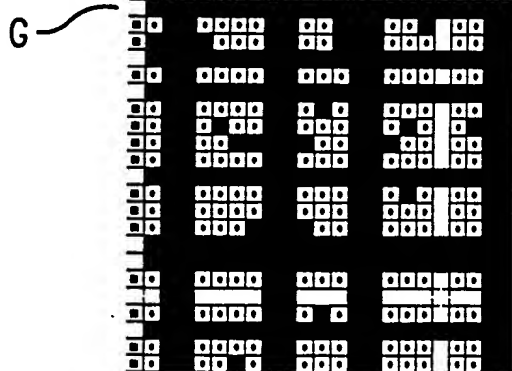
SYBYL: SPL SCRIPTS  
ON MSS

FIG.11(b)

FO5020" 8029260

BIOLOGICAL CRITERIA:  
METABOLICALLY HAZARDOUS  
BIOAVAILABILITY  
MOLECULAR WEIGHT  
CLOGP

SYBYL: SPL SCRIPTS ON  
MSS INVOKING -  
UNITY SEARCHES FOR  
FRAGMENTS  
CALCULATIONS OF MW  
& CLOGP



REMOVE NON-DIVERSE  
PRODUCTS:

GENERATE TANIMOTO  
2D FINGERPRINTS  
SAMPLE PRODUCTS:  
EXCLUDE TAN  $\geq 0.85$

## UNITY

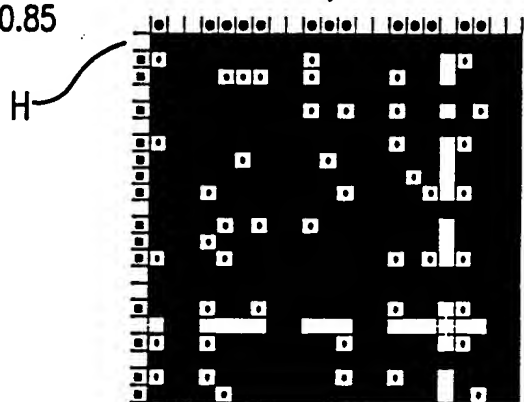
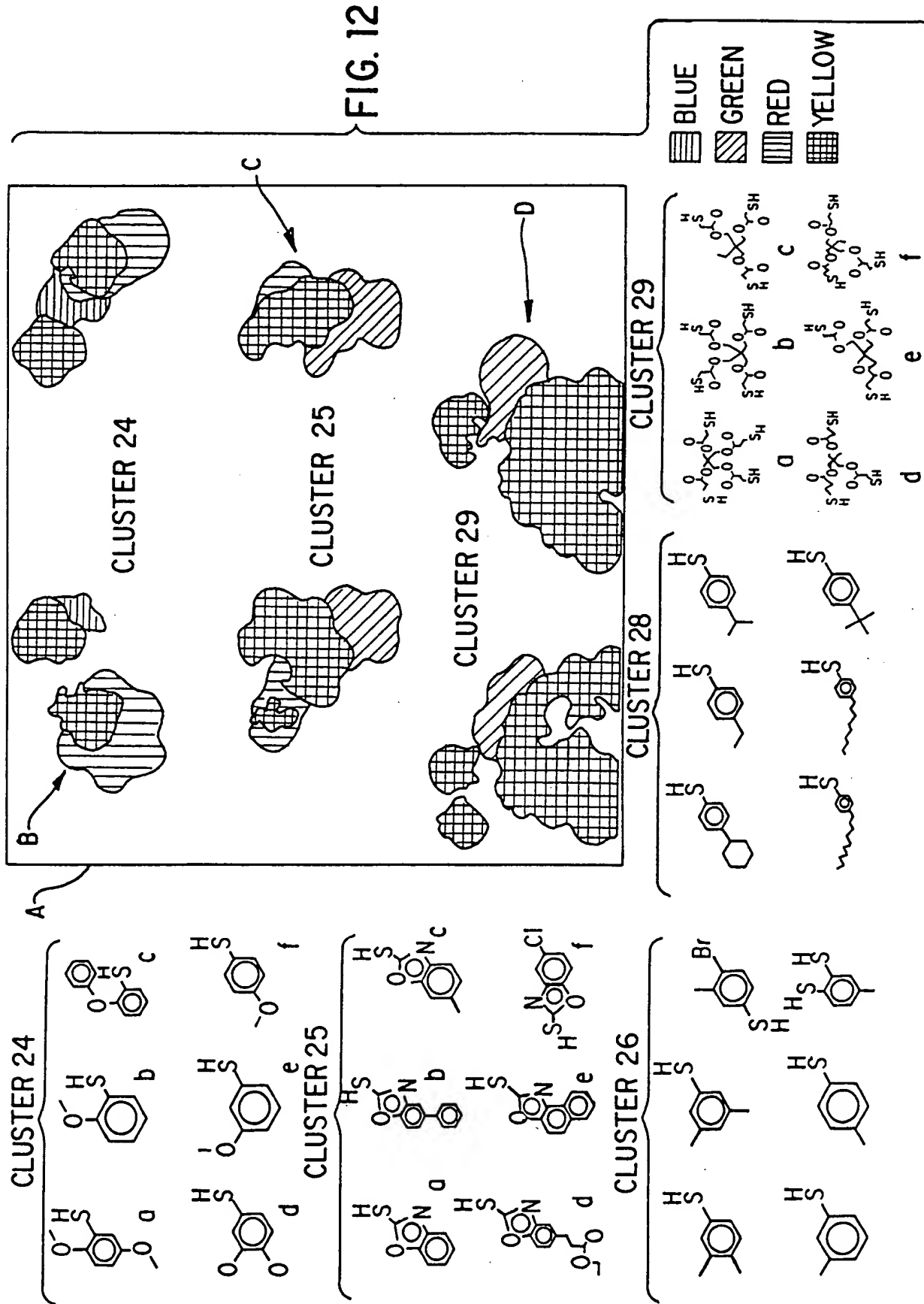


FIG. 11(c)

1. *Chlorophyll a* (Chl *a*)  
 2. *Chlorophyll b* (Chl *b*)  
 3. *Chlorophyll c* (Chl *c*)  
 4. *Chlorophyll d* (Chl *d*)  
 5. *Chlorophyll e* (Chl *e*)  
 6. *Chlorophyll f* (Chl *f*)  
 7. *Chlorophyll g* (Chl *g*)  
 8. *Chlorophyll h* (Chl *h*)  
 9. *Chlorophyll i* (Chl *i*)  
 10. *Chlorophyll j* (Chl *j*)  
 11. *Chlorophyll k* (Chl *k*)  
 12. *Chlorophyll l* (Chl *l*)  
 13. *Chlorophyll m* (Chl *m*)  
 14. *Chlorophyll n* (Chl *n*)  
 15. *Chlorophyll o* (Chl *o*)  
 16. *Chlorophyll p* (Chl *p*)  
 17. *Chlorophyll q* (Chl *q*)  
 18. *Chlorophyll r* (Chl *r*)  
 19. *Chlorophyll s* (Chl *s*)  
 20. *Chlorophyll t* (Chl *t*)  
 21. *Chlorophyll u* (Chl *u*)  
 22. *Chlorophyll v* (Chl *v*)  
 23. *Chlorophyll w* (Chl *w*)  
 24. *Chlorophyll x* (Chl *x*)  
 25. *Chlorophyll y* (Chl *y*)  
 26. *Chlorophyll z* (Chl *z*)  
 27. *Chlorophyll aa* (Chl *aa*)  
 28. *Chlorophyll ab* (Chl *ab*)  
 29. *Chlorophyll ac* (Chl *ac*)  
 30. *Chlorophyll ad* (Chl *ad*)  
 31. *Chlorophyll ae* (Chl *ae*)  
 32. *Chlorophyll af* (Chl *af*)  
 33. *Chlorophyll ag* (Chl *ag*)  
 34. *Chlorophyll ah* (Chl *ah*)  
 35. *Chlorophyll ai* (Chl *ai*)  
 36. *Chlorophyll aj* (Chl *aj*)  
 37. *Chlorophyll ak* (Chl *ak*)  
 38. *Chlorophyll al* (Chl *al*)  
 39. *Chlorophyll am* (Chl *am*)  
 40. *Chlorophyll an* (Chl *an*)  
 41. *Chlorophyll ao* (Chl *ao*)  
 42. *Chlorophyll ap* (Chl *ap*)  
 43. *Chlorophyll aq* (Chl *aq*)  
 44. *Chlorophyll ar* (Chl *ar*)  
 45. *Chlorophyll as* (Chl *as*)  
 46. *Chlorophyll at* (Chl *at*)  
 47. *Chlorophyll au* (Chl *au*)  
 48. *Chlorophyll av* (Chl *av*)  
 49. *Chlorophyll aw* (Chl *aw*)  
 50. *Chlorophyll ax* (Chl *ax*)  
 51. *Chlorophyll ay* (Chl *ay*)  
 52. *Chlorophyll az* (Chl *az*)  
 53. *Chlorophyll aza* (Chl *aza*)  
 54. *Chlorophyll abz* (Chl *abz*)  
 55. *Chlorophyll acz* (Chl *acz*)  
 56. *Chlorophyll adz* (Chl *adz*)  
 57. *Chlorophyll aez* (Chl *aez*)  
 58. *Chlorophyll afz* (Chl *afz*)  
 59. *Chlorophyll agz* (Chl *agz*)  
 60. *Chlorophyll ahz* (Chl *ahz*)  
 61. *Chlorophyll aiz* (Chl *aiz*)  
 62. *Chlorophyll ajz* (Chl *ajz*)  
 63. *Chlorophyll akz* (Chl *akz*)  
 64. *Chlorophyll alz* (Chl *alz*)  
 65. *Chlorophyll amz* (Chl *amz*)  
 66. *Chlorophyll anz* (Chl *anz*)  
 67. *Chlorophyll aoz* (Chl *aoz*)  
 68. *Chlorophyll apz* (Chl *apz*)  
 69. *Chlorophyll aqz* (Chl *aqz*)  
 70. *Chlorophyll arz* (Chl *arz*)  
 71. *Chlorophyll asz* (Chl *asz*)  
 72. *Chlorophyll atz* (Chl *atz*)  
 73. *Chlorophyll auz* (Chl *auz*)  
 74. *Chlorophyll avz* (Chl *avz*)  
 75. *Chlorophyll awz* (Chl *awz*)  
 76. *Chlorophyll axz* (Chl *axz*)  
 77. *Chlorophyll ayz* (Chl *ayz*)  
 78. *Chlorophyll ayz* (Chl *ayz*)  
 79. *Chlorophyll azz* (Chl *azz*)  
 80. *Chlorophyll azaa* (Chl *aza*)  
 81. *Chlorophyll abz* (Chl *abz*)  
 82. *Chlorophyll acz* (Chl *acz*)  
 83. *Chlorophyll adz* (Chl *adz*)  
 84. *Chlorophyll aez* (Chl *aez*)  
 85. *Chlorophyll afz* (Chl *afz*)  
 86. *Chlorophyll agz* (Chl *agz*)  
 87. *Chlorophyll ahz* (Chl *ahz*)  
 88. *Chlorophyll aiz* (Chl *aiz*)  
 89. *Chlorophyll ajz* (Chl *ajz*)  
 90. *Chlorophyll akz* (Chl *akz*)  
 91. *Chlorophyll alz* (Chl *alz*)  
 92. *Chlorophyll amz* (Chl *amz*)  
 93. *Chlorophyll anz* (Chl *anz*)  
 94. *Chlorophyll aoz* (Chl *aoz*)  
 95. *Chlorophyll apz* (Chl *apz*)  
 96. *Chlorophyll aqz* (Chl *aqz*)  
 97. *Chlorophyll arz* (Chl *arz*)  
 98. *Chlorophyll asz* (Chl *asz*)  
 99. *Chlorophyll atz* (Chl *atz*)  
 100. *Chlorophyll auz* (Chl *auz*)  
 101. *Chlorophyll avz* (Chl *avz*)  
 102. *Chlorophyll awz* (Chl *awz*)  
 103. *Chlorophyll axz* (Chl *axz*)  
 104. *Chlorophyll ayz* (Chl *ayz*)  
 105. *Chlorophyll ayz* (Chl *ayz*)  
 106. *Chlorophyll azz* (Chl *azz*)  
 107. *Chlorophyll azaa* (Chl *aza*)  
 108. *Chlorophyll abz* (Chl *abz*)  
 109. *Chlorophyll acz* (Chl *acz*)  
 110. *Chlorophyll adz* (Chl *adz*)  
 111. *Chlorophyll aez* (Chl *aez*)  
 112. *Chlorophyll afz* (Chl *afz*)  
 113. *Chlorophyll agz* (Chl *agz*)  
 114. *Chlorophyll ahz* (Chl *ahz*)  
 115. *Chlorophyll aiz* (Chl *aiz*)  
 116. *Chlorophyll ajz* (Chl *ajz*)  
 117. *Chlorophyll akz* (Chl *akz*)  
 118. *Chlorophyll alz* (Chl *alz*)  
 119. *Chlorophyll amz* (Chl *amz*)  
 120. *Chlorophyll anz* (Chl *anz*)  
 121. *Chlorophyll aoz* (Chl *aoz*)  
 122. *Chlorophyll apz* (Chl *apz*)  
 123. *Chlorophyll aqz* (Chl *aqz*)  
 124. *Chlorophyll arz* (Chl *arz*)  
 125. *Chlorophyll asz* (Chl *asz*)  
 126. *Chlorophyll atz* (Chl *atz*)  
 127. *Chlorophyll auz* (Chl *auz*)  
 128. *Chlorophyll avz* (Chl *avz*)  
 129. *Chlorophyll awz* (Chl *awz*)  
 130. *Chlorophyll axz* (Chl *axz*)  
 131. *Chlorophyll ayz* (Chl *ayz*)  
 132. *Chlorophyll ayz* (Chl *ayz*)  
 133.





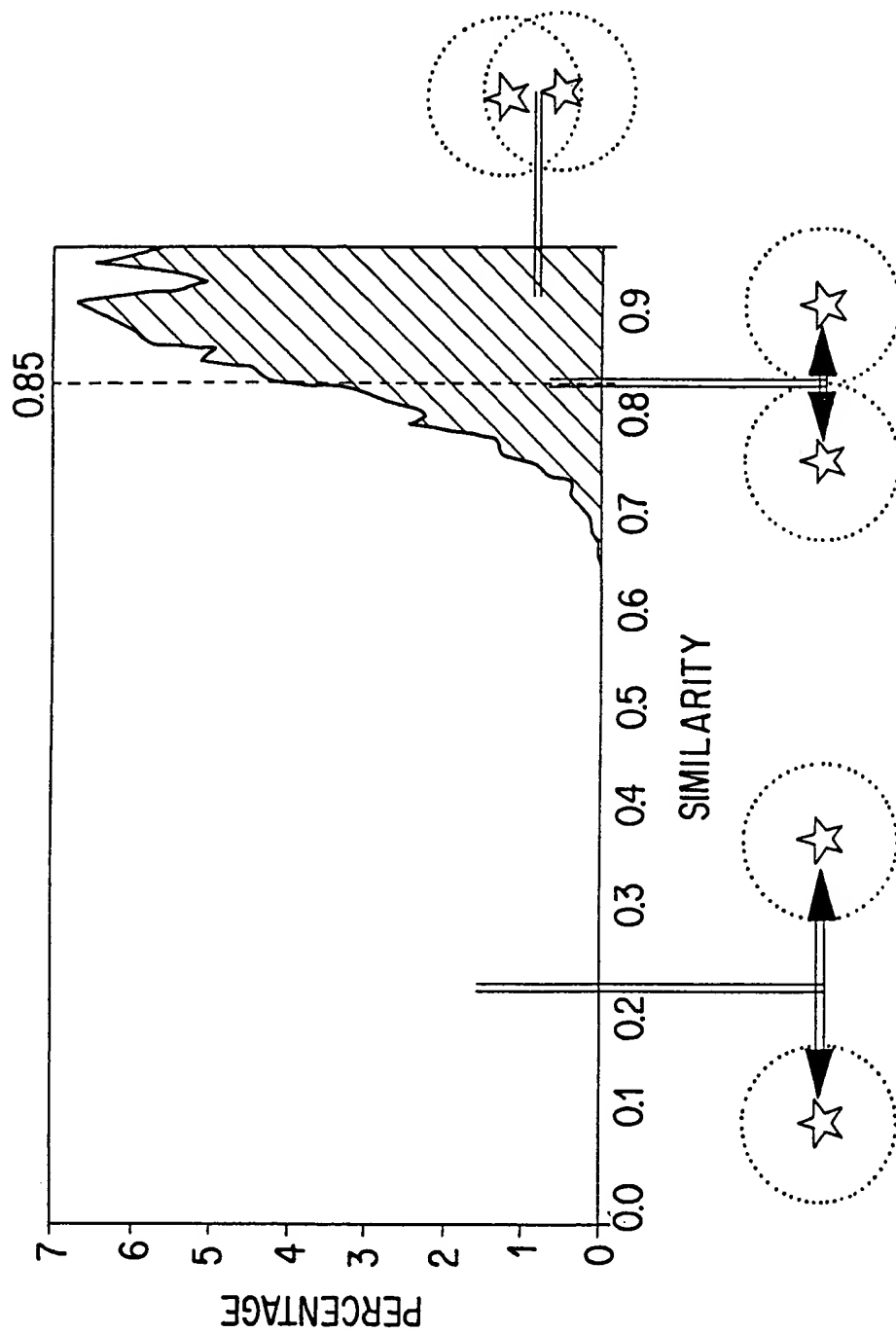


FIG.13

FIG. 14

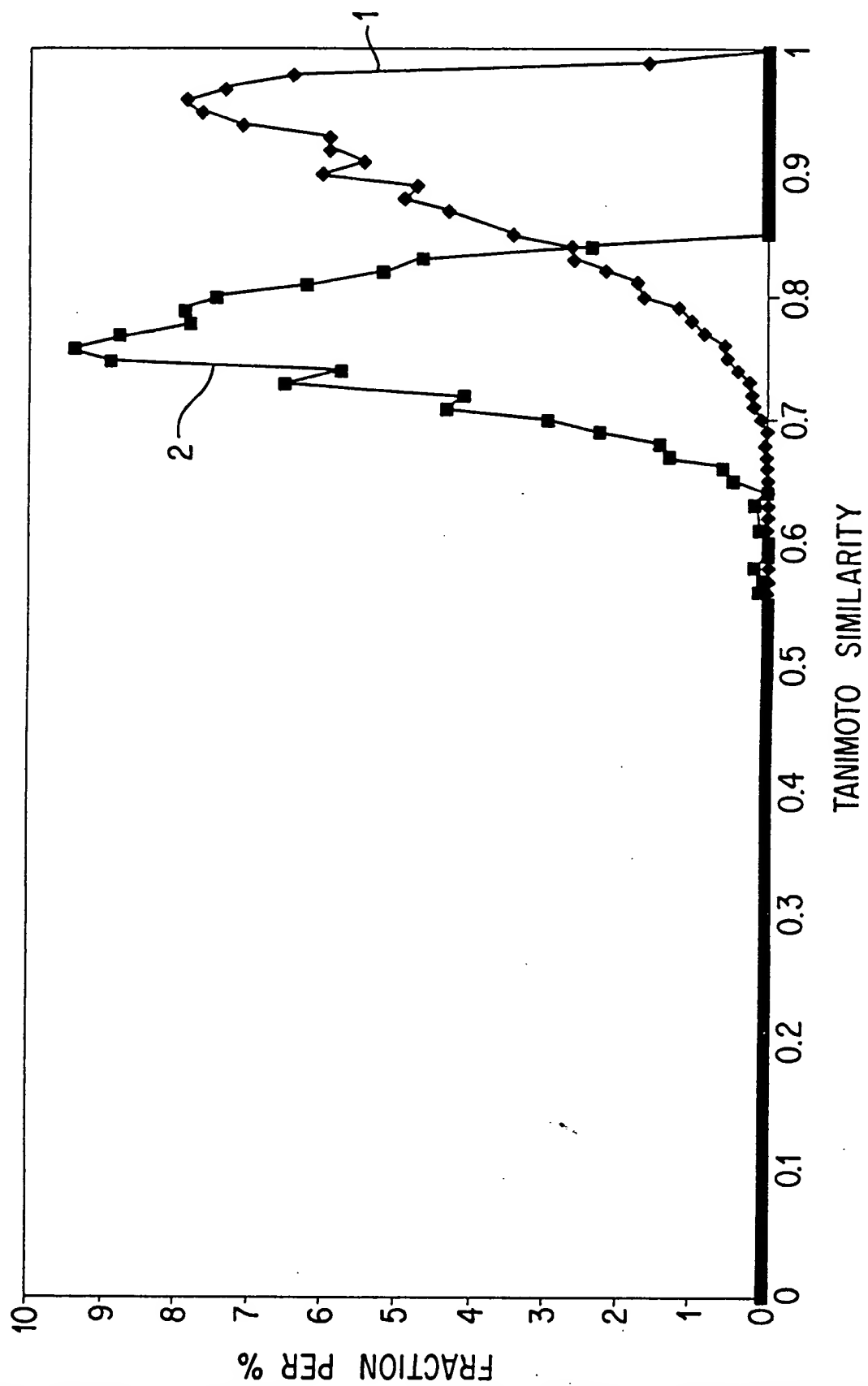


FIG.14

FO3020"8029260

